Shocks and slip systems: predictions from a theory of continuum dislocation dynamics

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(Dated: February 6, 2008)

Using a recently developed continuum theory of dislocation dynamics, we derive three new predictions about plasticity and grain boundary formation in crystals. (1) There will be a residual stress jump across grain boundaries and plasticity-induced cell walls, which self-consistently acts to form the boundary by attracting neighboring dislocations; we derive the asymptotic late-time dynamics of the grain-boundary formation process. (2) At grain boundaries formed at high temperatures, there will be a cusp in the elastic energy density. (3) In early stages of plasticity, when only one type of dislocation is active (single-slip stage I plasticity), cell walls will not form; instead we predict the formation of jump singularities in the dislocation density.

PACS numbers: 46.,91.60.Dc,91.60.Ed,47.40.-x

Dislocation motion governs the plastic deformation of crystals, as well as the formation and evolution of grain boundaries in polycrystals. Acharya and Roy [1] recently proposed an evolution law for the density of dislocations in crystals, allowing both glide and climb (hence appropriate at high temperatures). We subsequently rederived this law from the microscopic dynamics and a closure approximation, proposed a modified law to suppress climb, and showed numerically that both laws developed shock singularities [2]. We argued that these shocks are the fundamental origin of the wall-like structures spontaneously formed by dislocations—providing a continuum explanation of both the grain boundaries formed at high temperatures and the cell walls formed at low temperatures in plastically deformed crystals. Wall formation thus emerges naturally from this continuum formulation. What other properties and predictions naturally emerge from this mesoscale perspective? Here we discuss three.

(1) *Residual stress.* The continuum model predicts residual stresses associated with the formation of grain boundaries and cell walls. It makes detailed predictions about the asymptotic behavior of the stress and dislocation density near the walls, and about how the wall's associated stress allows it to draw in and absorb neighboring dislocations.

(2) *Cusps in energy density.* The continuum model predicts that the elastic energy associated with the residual stress is continuous across a grain boundary (despite the jumps in the individual stress components). The energy density does have a cusp singularity.

(3) *Dislocation density jumps in single-slip.* When appropriately restricted to forbid climb, the model predicts that materials with only one kind of dislocation will not form cell walls, explaining the lack of such structures in systems (discrete-dislocation simulations and experimental stage I plasticity) where only one slip system is active. Instead, the model predicts that these systems will form a more subtle jump singularity in the dislocation density.

We will derive these three predictions analytically by mapping the dislocation dynamics theory in one dimension onto *Burgers equation.* We will present numerical simulations to flesh out these predictions. Finally, we will consider how and whether these predictions are likely to depend upon the detailed structure of the continuum model, and how physical mechanisms ignored by the model will likely affect and modify these striking predictions. We begin by introducing our notation and Acharya and Roy's derivation of the equations of motion we study.

A complete macroscopic description of the deformation $\mathbf{u}$ of a material is given by $\partial_i u_j = \beta^{\mathrm{E}}_{ij} + \beta^{\mathrm{P}}_{ij}$, where β^{E}_{ij} represents the elastic, reversible distortion and the plastic distortion tensor β^{P}_{ij} describes the irreversible plastic deformation. The plastic distortion is the result of the net density of dislocations, described by the Nye dislocation density tensor [3, 4, 5, 6, 7]

$$\rho_{ij}(\mathbf{x}) = -\varepsilon_{ilm}\partial_l \beta^{\mathrm{P}}_{mj} = \sum_\alpha t^\alpha_i b^\alpha_j \delta(\boldsymbol{\xi}^\alpha) \qquad (1)$$

which measures the net flux of dislocation α, tangent to $\mathbf{t}$, with Burgers vector $\mathbf{b}$, in the (coarse-grained) neighborhood of $\mathbf{x}$.

The time evolution of the plastic distortion tensor is given in terms of a function $J_{ij} = \partial_t \beta^{\mathrm{P}}_{ij}$, where $\varepsilon_{ilm}J_{mj}$ gives the net current for the conserved Burgers vector of the dislocation density tensor, $\partial_t \rho_{ij} = -\varepsilon_{ilm}\partial_l J_{mj}$. The current from a single dislocation moving with velocity $\mathbf{v}$ is $J_{ij} = \varepsilon_{iln} t_l b_j v_n \delta(\boldsymbol{\xi})$, and the net Peach–Koehler force on a dislocation driving its motion is $f^{\mathrm{PK}}_l = -\varepsilon_{lmn} t_m b_c \sigma_{nc}$ where $\boldsymbol{\sigma}$ is the local stress (due, for example, to the other dislocations). In our derivation of the equation of motion [2], we allowed each dislocation to move independently, and then made a closure approximation to write $\boldsymbol{J}$ in terms of $\boldsymbol{\rho}$. Roy and Acharya [1] got the same final result by simply assuming that all the dislocations move with the same velocity $\mathbf{v}$, given by a constant $(D(\rho)/2)$ times the force density $\mathcal{F}_l = -\varepsilon_{lmn}\rho_{mc}\sigma_{nc}$ on the local

dislocations:

$$J_{ij}^{\mathrm{RA}} = \frac{D}{2}\,\varepsilon_{ial}\mathcal{F}_l\rho_{aj} = -\frac{D}{2}\,\varepsilon_{ial}(\varepsilon_{lmn}\rho_{mc}\sigma_{nc})\rho_{aj} = \frac{D}{2}(\sigma_{ic}\rho_{ac} - \sigma_{ac}\rho_{ic})\rho_{aj}. \tag{2}$$

A physically natural choice for $D(\rho)$ is proportional to an inverse density of dislocation lines (so that the force per dislocation drives the motion [1]); we choose here to discuss the mathematically more convenient choice of a constant D. (Numerically, both give qualitatively similar evolution [2].) We controlled the microscopic mobility difference between glide and climb [2] by introducing a mesoscale parameter λ. By setting

$$\partial_t \beta_{ij}^{\mathrm{P}} = J_{ij} = J_{ij}^{\mathrm{RA}} - \frac{\lambda}{3}\,\delta_{ij} J_{kk}^{\mathrm{RA}}, \tag{3}$$

at low temperatures $\lambda = 1$ removed the trace of $\boldsymbol{J}$ enforcing volume conservation, and hence forbids climb, while at high temperatures $\lambda = 0$ allowed for equal mobilities for both glide and climb.

We now turn to an analysis of the continuum equation in one dimension. Near a wall singularity (say, perpendicular to $\hat{\mathbf{z}}$) the dynamics is one-dimensional. The variations of the stress, plastic strain, and dislocation densities parallel to the wall asymptotically become unimportant compared to the variations along $\hat{\mathbf{z}}$ as one approaches the singularity. In one dimension the stress $\boldsymbol{\sigma}(\mathbf{x})$, generally given by a long-range integral over the neighboring dislocations $\boldsymbol{\rho}(\mathbf{x}')$, can be written as a linear function of the local plastic distortion $\boldsymbol{\beta}^{\mathrm{P}}$:

$$\sigma_{ij} = -\bar{C}_{ijkm}\beta_{km}^{\mathrm{P}} \tag{4}$$

where

$$\bar{C}_{ijkm} = \mu\left(\bar{\delta}_{ik}\bar{\delta}_{jm} + \bar{\delta}_{im}\bar{\delta}_{jk} + \frac{2\nu}{1-\nu}\,\bar{\delta}_{ij}\bar{\delta}_{km}\right) \tag{5}$$

(not quite equal to the elasticity tensor), and the Kronecker delta is modified such that $\bar{\delta}_{zz} = 0$. Hence the evolution law for $\boldsymbol{\beta}^{\mathrm{P}}$ simplifies dramatically. The β_{zj}^{P} components do not evolve (except β_{zz}^{P} for $\lambda \neq 0$, which helps enforce volume conservation); the other components all evolve according to

$$\partial_t \beta_{ij}^{\mathrm{P}} = -\frac{1}{2}(\partial_z \mathcal{E})\,\partial_z\left(\beta_{ij}^{\mathrm{P}} - \frac{\lambda}{3}\,\beta_{kk}^{\mathrm{P}}\delta_{ij}\right) \tag{6}$$

where we have rescaled the time to set $D = 1$. The elastic energy density $\mathcal{E}$ in equation 6 can be written in terms of the local plastic distortion tensor:

$$\mathcal{E} = \frac{1}{2}\,\bar{C}_{ijkm}\beta_{ij}^{\mathrm{P}}\beta_{km}^{\mathrm{P}} = \frac{\mu}{2}(\beta_{xy}^{\mathrm{P}} + \beta_{yx}^{\mathrm{P}})^2 + \mu\left({\beta_{xx}^{\mathrm{P}}}^2 + {\beta_{yy}^{\mathrm{P}}}^2\right) + \frac{\mu\nu}{1-\nu}(\beta_{xx}^{\mathrm{P}} + \beta_{yy}^{\mathrm{P}})^2 \tag{7}$$

We now specialize to the case of $\lambda = 0$, where glide and climb are treated on an equal footing (applicable to grain boundary formation during polygonization at high temperatures, for example). In this case, equation 6 tells us that the individual components of $\boldsymbol{\beta}^{\mathrm{P}}$ are all independent of one another, slaves solely to the evolution of the total stress energy density $\mathcal{E}$. By contracting equation 6 with $\bar{C}_{ijkm}\beta_{km}^{\mathrm{P}}$ then using expression 7, the time evolution of the strain energy becomes

$$\partial_t \mathcal{E} + \frac{1}{2}\,(\partial_z \mathcal{E})^2 = 0\,. \tag{8}$$

Equation 8 can be cast into the famous Burgers equation by defining $\mathcal{F} = \partial_z \mathcal{E}$ [8, 9, 10]:

$$\partial_t \mathcal{F} + \mathcal{F}\partial_z \mathcal{F} = 0. \tag{9}$$

The scalar $\mathcal{F}(z)$ is again the net Peach–Koehler force density on the local dislocation density $\boldsymbol{\rho}(z)$. Burgers equation is the archetype of hyperbolic partial differential equations. Under Burgers equation $\mathcal{F}$ will develop sharp jumps downward after a finite evolved time, corresponding to cusps in the energy density $\mathcal{E}$ and leading to jumps in the components of $\boldsymbol{\beta}^{\mathrm{P}}$ (Fig 1).

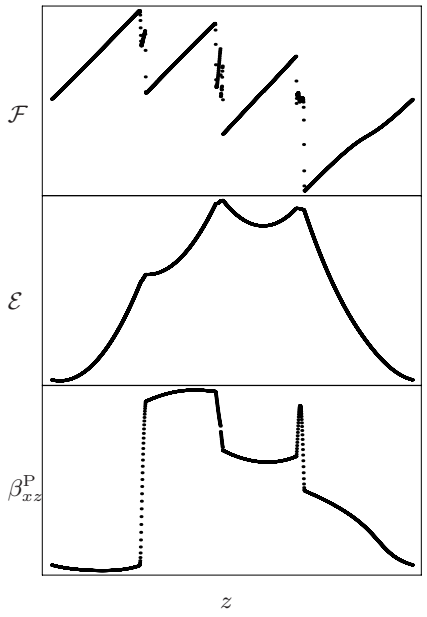

FIG. 1: **Cusps and jumps in one dimension.** For the continuum dynamics equation allowing both glide and climb, the Peach–Koehler force density $\mathcal{F}$ obeys Burgers equation, and hence develops sharp jumps (top). The individual components of the plastic distortion tensor $\boldsymbol{\beta}^{\mathrm{P}}$ (bottom), as well as the stress and strain tensors, evolve to also have sharp jumps at the walls; the dislocation density hence develops the δ-function singularity associated with grain boundary formation. These discontinuities in the residual stresses and strains, however, cancel out in the net elastic energy density, which is continuous with only a cusp at the walls (middle).

At late times, the asymptotic late-time solutions to Burgers equation (between the singularities) are linear

functions of z whose slopes decay with time:

$$\mathcal{F} \sim \frac{z - z_0}{t - t_0} \tag{10}$$

The corresponding elastic energy density (continuous across the singularities) has asymptotic form given by integrating equation 10:

$$\mathcal{E} \sim \frac{1}{2}\frac{(z - z_0)^2}{(t - t_0)} + \mathcal{E}_0 \tag{11}$$

The individual components of the distortion tensor (apart from the three time-independent components β_{zj}) numerically take the form

$$\beta^{\mathrm{P}}_{ij} \sim \alpha_{ij}\frac{z - z_0}{\sqrt{t - t_0}} + \gamma_{ij}\,, \tag{12}$$

which can be shown to be consistent with the evolution law for the energy density (equation 11), so long as the coefficients α_{ij} and γ_{ij} obey the relations

$$\begin{gathered}\bar{C}_{ijkm}\alpha_{ij}\alpha_{km} = 1\,, \qquad \bar{C}_{ijkm}\alpha_{ij}\gamma_{km} = 0\,, \\ \bar{C}_{ijkm}\gamma_{ij}\gamma_{km} = 2\mathcal{E}_0\,,\end{gathered} \tag{13}$$

for $i, j = x$ or y; there are no restrictions on α_{iz} and γ_{iz}.

There has been extensive work on discrete point dislocation simulations in two dimensions, where it appears necessary to include more than one slip system to form walls [11, 12, 13, 14, 15, 16, 17, 18]. What does the continuum model predict for this case? Let us consider a 2D system (constant along $\hat{\mathbf{z}}$) of straight edge dislocations with Burgers vector along $\hat{\mathbf{x}}$, described by a single non-zero component $\rho_{zx}(x, y)$. Such a system has two non-zero components of the distortion tensor, $\rho_{zx} = -\partial_x\beta^{\mathrm{P}}_{yx} + \partial_y\beta^{\mathrm{P}}_{xx}$.

A simulation of this system with Gaussian random initial β^{P}_{yx} and β^{P}_{xx}, allowing both glide and climb, generates a series of walls of dislocations roughly parallel to the $\hat{y}$-axis similar to those seen by Barts and Carlsson [19] in their 2D study of single slip with both glide and climb. (See figure 3.)

To forbid climb in this case it is convenient [22] to simply choose $\beta^{\mathrm{P}}_{xx} \equiv 0$. Figure 2 shows the evolution of the distortion field for climb-free dynamics with a single slip system. In agreement with experiment and the discrete dislocation simulations [20, 21], we observe no cell wall structures in single slip (which would correspond to jumps in $\boldsymbol{\beta}^{\mathrm{P}}$ in Fig 2). Instead, we find a network of surfaces exhibiting a striking new singularity: a cusp in the distortion tensor, corresponding to a jump in the dislocation density. We can understand this singularity analytically using our mapping to Burgers equation. With only one non-zero component of $\boldsymbol{\beta}^{\mathrm{P}}$, the energy density is proportional to the square of β^{P}_{yx} (eqn 7). The energy density satisfies eqn 8 and forms cusps, so the distortion tensor must also form cusps.

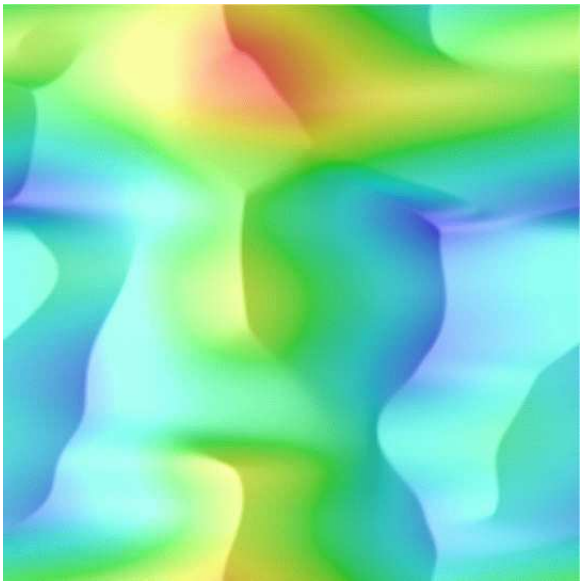

FIG. 2: **Cusps formed with one slip system.** Plastic distortion tensor β^{P}_{yx} formed by climb-free evolution of a Gaussian random initial state of edge dislocations pointing along $\hat{\mathbf{z}}$ with Burgers vector along $\pm\hat{\mathbf{x}}$. Notice that walls do not form with one slip system, only cusps in the distortion tensor; compare to [21].

Which of these new predictions of the mesoscale dislocation dynamics model can be trusted? Which seem (in retrospect) physically plausible, and which are likely artifacts of simplifications made in the modeling process, or just mathematical curiosities of this particular model?

(1) *Residual stress.* The primary driving force for dislocation motion is stress. In cases where dislocations dynamically assemble into walls (polygonization at high temperatures, cell wall formation at low temperatures), it does seem natural in retrospect to expect that the walls will be associated with stress jumps designed to attract residual dislocations to the walls. Grain boundaries formed from the melt when separate growing crystals touch should likely not be described by the continuum model [23]. These residual stress jumps must be viewed as a fundamental prediction of the model.

(2) *Cusps in the energy density.* If there are jumps in the stress at grain boundaries, surely it is natural that there be some singularity in the energy density. At late stages when the dislocations between grain boundaries have all been removed, a flat boundary can lower the system energy by moving into the region of higher energy density. If both glide and climb are allowed [24], and if dislocation mobility is unimpeded (by precipitates, impurities, lattice pinning, or tangling) this traction will lead the boundaries to move until the energy density is continuous across the boundary. Hence, for mobile walls at high temperatures, it is natural to expect the energy density to be continuous, and have only cusp singulari-

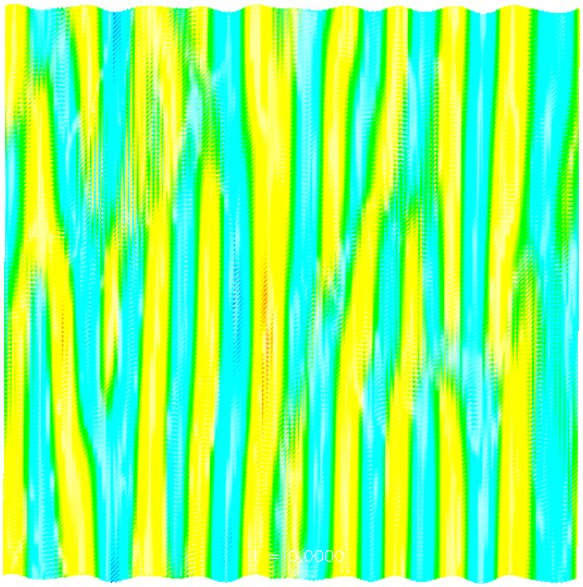

FIG. 3: **Continuum of walls.** The dislocation density tensor ρ_{zx} evolved allowing both glide and climb from a random initial state of edge dislocations along $\mathbf{t} \sim \hat{\mathbf{z}}$ with $\mathbf{b} \sim \hat{\mathbf{x}}$. Notice that the dislocations arrange themselves into small-angle tilt boundaries at the lattice scale, but do not coarsen; compare to [19].

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(3) *Dislocation density jumps in single-slip.* The formation of dislocation walls in the continuum theory cannot properly be called a prediction, since wall formation is well known experimentally. It is, however, a natural consequence of the hyperbolic form of the equations. The (hitherto unobserved) prediction of dislocation density jumps in early stages of plasticity when only one slip system is active is also a natural consequence of hyperbolic equations. Our continuum model is guaranteed to lower the net energy with time, reassuring us that the predicted dislocation density jumps are energetically favorable and satisfy all compatibility constraints. They could, however, be smeared by pinning and inhomogeneities in real systems just as grain boundaries and cell walls are distorted by these effects. A smeared dislocation density jump may be more challenging to identify than a smeared wall of dislocations, perhaps explaining why these jumps have not yet been seen experimentally.

We thus predict that residual stress is not due to inhomogeneities or other infelicities in the formation process, but is an intrinsic component of the formation of grain boundaries and cell walls. We make concrete predictions about the nature and form of these stresses near grain boundaries, that should be testable in colloidal systems or using next-generation X-ray sources. We provide a mesoscale explanation for one of the key morphological distinctions between early (stage I) and later (stage III) plasticity. Finally, we predict a new *dislocation density jump* structure in plastically deformed systems with only one active slip system.

We thank Amit Acharya for helpful conversations, and acknowledge funding from NSF grants ITR/ASP ACI0085969 and DMR-0218475.

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[22] Our proposed evolution law equation 3 suppressed climb by removing the trace of the current, hence the term $-\lambda/3\, J_{kk}\delta_{ij}$ in $\partial_t \beta^{\mathrm{P}}_{ij}$. This choice is inconvenient here, because it introduces new components β^{P}_{yy} and β^{P}_{zz} to the problem, and the corresponding dislocation densities ρ_{zy}, ρ_{xz}, and ρ_{yz}. While these are allowed by symmetry, they are not part of the discrete dislocation simulation.
[23] One concern we have is that a wall with a stress jump can lower its energy by splitting in two; stress jumps at walls in real materials may be stabilized by a different mechanism than in the continuum model.

[24] The glide-only continuum model does have small jumps in the energy density.